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Extraction of Modeling Parameters for Low-Loss Alternative Plasmonic Material

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Abstract

Plasmonics is a revolutionary branch of photonics which offers the benefit of both nanoscale electronics and broadband photonics by coupling the photon energy and momentum to free electron gas on the surface of metals generating a quasi-particle wave known as surface plasmon which enables the manipulation of light at the nanoscale. Though metals are the basic building blocks of plasmonic devices, they are blighted by high resistive losses at optical frequencies which restrict the development of surface plasmon based devices. This calls for the development of alternative materials for plasmonic applications. Transparent conducting oxides such as aluminum zinc oxide (AZO) and gallium zinc oxide (GZO) behave like metals in the near Infra-Red region which enables the application of these materials as alternatives to metals in plasmonic devices. The advantages include low intrinsic loss, tunability, compatibility with semi-conductor based design and fabrication methods etc. In order to simulate the performance of these materials as plasmonic materials, the modeling parameters need to be found out. In this paper we report the Drude and Lorentz model parameters for AZO and GZO. The modeling parameters have been extracted using a nonlinear optimization algorithm. In order to validate the optimized parameters we have determined the complex relative permittivity using the extracted parameters and compared them with the experimental results and an excellent agreement has been found. The root-mean-square (RMS) deviations are found to be as little as 0.0259 and 0.0479 for Drude model and 0.0680 and 0.0587 for Lorentz model respectively for AZO and GZO. It is expected that the modeling parameters will be of great use to the plasmonics research community for the development of new devices.

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Keywords: Plasmonic material; Lorentz model; Drude model; Nelder Mead method

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1. Introduction

Rapid advancement in optical nano technology and plasmonics have stimulated considerable interest in metal and dielectric nanostructures in wide range of applications such as bio-sensing (Sagor, Saber, Al-Amin, & Al Noor, 2013), Bragg reflectors (Hosseini & Massoud, 2006), sub-wavelength imaging (Melville & Blaikie, 2005), metamaterials (Henzie, Lee, & Odom, 2007) and enhanced light absorption in solar cell (Chou & Ding, 2013), owing to their unique optical properties. In particular, research on plasmonics has attracted a lot of research importance due to its capability to overcome the diffraction limit (Barnes, Dereux, & Ebbesen, 2003; Maier, 2007; M. Saber, Sagar, Al-Amin, & Noor, 2013).

Plasmonics involves the study of interaction between electromagnetic fields and free electrons in metal. The electric component of light can stimulate the free electrons in the metal to have collective oscillations. Metals are essential for creating surface plasmon polariton (SPP). In order to simulate real plasmonics materials using finite difference time domain (FDTD) method (Yee, 1966), it is required to incorporate the formulations of frequency dependent properties of materials in the simulation model. Several methods have been reported to model the frequency dependent properties of the optical materials. The metal-dielectric-metal parameters for gold in the wavelength range of 550-950 nm is presented by Jin et al (Jin & Xu, 2006). Krug et al. modelled the gold parameters that are valid in the wavelength range of 700-1000 nm (Krug II, Sánchez, & Xie, 2002). W.H.P. Pernice et al. (Pernice, Payne, & Gallagher, 2007) used Lorentz-Drude model to extract the parameters for Nickel. Parameters for Nickel, Palladium, Titanium and 8 other metals using Lorentz-Drude and Brendel-Bormann Model were reported by A.D. Rakic et al. (Rakic, Djurišić, Elazar, & Majewski, 1998). R. H. Sagor et al. used modified Debye model to extract the parameters for several metals (M. G. Saber & Sagor, 2013b; Sagor, et al., 2013).

However, the plasmonic devices available at present face considerable challenge because of the losses encountered in the constituent metals. Losses are inevitable for the plasmon oscillation due to the ohmic loss and electron core interaction (Maier, 2007). The practical applications of the materials are restricted by these losses. A number of comparative researches are being conducted in order to find out new low loss plasmonic materials that can provide enhanced propagation of the SPP and support better confinement for the SPP mode. A detailed comparison on different plasmonic materials was reported by P. R. West et al (West et al., 2010) where the essential aspects of fabrication were analysed. W. Guo et al (Guo et al.) used silver metal to present an analysis of symmetric SPP mode propagation in Ag/Al₂O₃/Ag waveguide. Similar type of SPP mode propagation was investigated by M. G. Saber et al. using Ag thin film in Dielectric-Metal-Dielectric (DMD) waveguide (M. Saber, et al., 2013; M. G. Saber & Sagor, 2013a). Metal shows the negative electric permittivity $\epsilon_m(\omega)$ naturally in certain range of wavelength that is described by the Drude electron model in metals (Ramakrishna, 2005). Though the metal involvement causes consistent energy losses in plasmonic propagation, metals are being used due to the presence of natural negative permittivity property.

In this paper, we report the extraction of optimized parameter of two new transparent conducting oxide AZO and GZO for Drude and Lorentz model with the goal of reducing the propagation loss of plasmonic materials. The equations describing the two models are nonlinear in nature. AZO and GZO behave like metals in the near Infra-Red region which enables the application of these materials as alternatives to metals in plasmonic devices. The optical characteristics of AZO and GZO films exhibit considerably lower loss than Ag at telecommunication wavelengths (Hiramatsu, Imaeda, Horio, & Nawata, 1998; Kim et al., 2000; West, et al., 2010) which are of certain importance for plasmonics applications. The losses of AZO and GZO are found to be more than three times lower than the silver at 1.5 μm wavelength. In this work, a nonlinear algorithm is developed to optimize the material modelling parameters for the two models. In order to validate the optimized parameters we have determined the complex relative permittivity using the extracted parameters and compared them with the experimental results (West, et al., 2010) and an excellent agreement has been found. The root-mean-square (RMS) deviations are found to be as little as 0.0259 and 0.0479 for Drude model and 0.0680 and 0.0587 for Lorentz model respectively for AZO and GZO. This study will help the researchers to represent the materials in a more accurate manner and develop realistic simulation models that will, as a consequence, be responsible for accurate results.

2. Material Models

2.1. Lorentz Model

The frequency dependent complex permittivity function of multi-pole Lorentz model (Alsunaidi & Al-Jabr, 2009; Kunz & Luebbers, 1993) is given by,

$$\varepsilon_r(\omega) = \varepsilon_\infty + \sum_{p=1}^P \frac{\Delta\varepsilon_p \omega_p^2}{\omega_p^2 + j2\delta_p \omega - \omega^2} \dots\dots\dots (1)$$

where, ε_∞ is the infinite frequency relative permittivity, j is the imaginary unit, δ is the damping coefficient, ω_o is the frequency of the pole pair, P is the number of Lorentz pole pair and the change in relative permittivity due to the p^{th} pole pair is represented by $\Delta\varepsilon_p$. It can be observed from equation (1) that multi-pole Lorentz model can be described by four parameters of ε_∞ , $\Delta\varepsilon_p$, δ_p and ω_p . These four parameters are independent and needed to be optimized if we want to model any material using Lorentz model.

2.2. Drude Model

The frequency dependent permittivity function of single pole Drude model (Ordal et al., 1983) is given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\Delta\varepsilon\omega_o^2}{j2\delta\omega - \omega^2} \dots\dots\dots (2)$$

where, ε_∞ is the infinite frequency relative permittivity, j is the imaginary unit, δ is the damping coefficient, ω_o is the frequency of the pole pair, and the change in relative permittivity is represented by $\Delta\varepsilon$. It can be observed from equation (2) that multi-pole Drude model can be described by four parameters of ε_∞ , $\Delta\varepsilon$, δ and ω_o . These four parameters are independent and need to be optimized if we want to model any material using Drude model.

3. Optimization Method

A nonlinear optimization algorithm based on the Nelder Mead method has been developed in order to extract the parameters. The frequency dependent complex permittivity of any material can be expressed in terms of its real and imaginary part as, $\varepsilon_r(\omega) = \varepsilon_{real} + j\varepsilon_{img}$. The experimental values of real ε_{real} and imaginary ε_{img} parts of complex permittivity were obtained from (West, et al., 2010).

A group of guess values of the parameters which need to be optimized is provided. The complex relative permittivity is calculated by inserting the guess values into the mathematical model. The next task is to develop an objective function which would calculate the deviation of the calculated permittivity from the experimental one. Then the objective function has to be minimized by varying the parameters so that the deviation becomes smaller in successive iterations and ultimately comes down to a predefined tolerance level.

We defined the objective function as follows:

$$f(\varepsilon_\infty, \Delta\varepsilon_p, \delta_p, \omega_p) = \sqrt{\sum (x_1^2 + x_2^2)} \dots\dots\dots (3)$$

where

$$x_1 = \varepsilon_{real_calc}(\varepsilon_\infty, \Delta\varepsilon_p, \delta_p, \omega_p) - \varepsilon_{real_ex}(\varepsilon_\infty, \Delta\varepsilon_p, \delta_p, \omega_p) \dots\dots\dots (4)$$

$$x_2 = \varepsilon_{img_calc}(\varepsilon_\infty, \Delta\varepsilon_p, \delta_p, \omega_p) - \varepsilon_{img_ex}(\varepsilon_\infty, \Delta\varepsilon_p, \delta_p, \omega_p) \dots\dots\dots (5)$$

where ε_{real_calc} is the real part of permittivity calculated using the obtained parameters, ε_{real_ex} is the experimentally obtained real part of permittivity, ε_{img_calc} is the calculated imaginary part of permittivity, ε_{img_ex} is the experimentally obtained imaginary part of permittivity.

The Nelder Mead algorithm, also known as the ‘Amoeba algorithm’, was used for minimizing the objective function. Like Genetic algorithms (GA), the Nelder Mead algorithm advances iteratively by modifying a group of possible solutions till they converge to a single optimal solution. The method involves 5 major steps- initialization, reflection, expansion, contraction and shrinking. These steps are discussed in detail in (Dennis & Woods, 1987; Kelley, 1999)

4. Results and Discussion

The parameters extracted using the nonlinear optimization algorithm are presented in Table 1 and Table 2. The curves for real and imaginary parts of the complex relative permittivity are shown for both optimized and experimental values. The applicable wavelength range and the RMS deviations are also presented. Table 1 shows the optimized parameters for AZO and GZO for single pole pair Drude model. The maximum RMS deviation for AZO and GZO are found to be 0.0259 and 0.04796 respectively when single pole pair Drude model is used.

Table 1. Optimized parameters for AZO and GZO for single pole pair Drude model.

Parameters	AZO	GZO
ε_∞	4.0924	4.089504
$\Delta\varepsilon$	0.0259	0.018821
δ (rad/sec)	8.4823e+013	1.3948e+014
ω_o (rad/sec)	1.8186e+016	2.1262e+016
Range of wavelength (nm)	520-2080	520-2150
RMS deviation	0.0259	0.04796

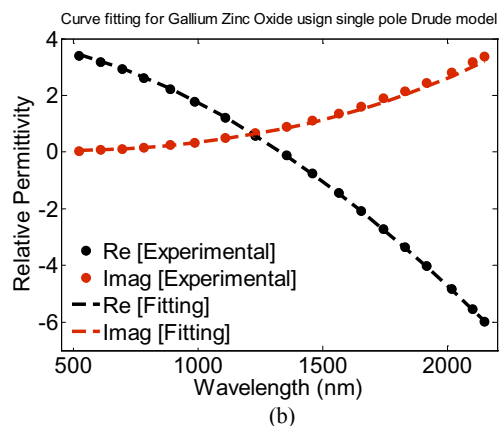
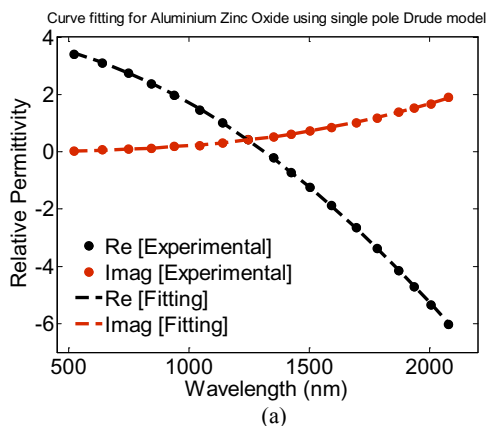


Fig. 1 Comparison between the real and the imaginary parts of the complex relative permittivity obtained using both extracted parameters for Drude model and experimental values for (a) AZO (b) GZO

Table 2 shows the optimized parameters for AZO using three pole Lorentz model and GZO using four pole Lorentz model. The Lorentz model gives maximum RMS deviation of 0.068 and 0.0587 for AZO and GZO respectively. The range of applicable wavelengths are 520nm-2080nm and 520nm-2150nm for AZO and GZO respectively. From the tables it can be seen that the parameters can be applied for a wide range of wavelengths. The comparisons between the experimental values and the obtained results have been graphically shown in Fig. 1 and Fig. 2 for the single-pole Drude model and the multi pole Lorentz model respectively. The figures show very good agreement between the experimental and the optimized curve.

Table 2. Optimized parameters for AZO and GZO for multi pole pair Lorentz model.

Parameters	AZO	GZO
ϵ_{∞}	1	1
$\Delta\epsilon_1$	2.764019	94.2957
$\Delta\epsilon_2$	100	-11.3683
$\Delta\epsilon_3$	-0.375971	75.8960
$\Delta\epsilon_4$	N/A	-108.1021
δ_1 (rad/sec)	6.4088e+13	-4.9933e+18
δ_2 (rad/sec)	7.9168e+13	-1.4171e+20
δ_3 (rad/sec)	7.7643e+18	1.1770e+17
δ_4 (rad/sec)	N/A	4.1469e+20
ω_1 (rad/sec)	1.0438e+16	9.6769
ω_2 (rad/sec)	2.7708e+14	5.0133
ω_3 (rad/sec)	5.1862e+16	-1.1862
ω_4 (rad/sec)	N/A	6.5525
Range of wavelength (nm)	520-2080	520-2150
RMS deviation	0.0680	0.0587

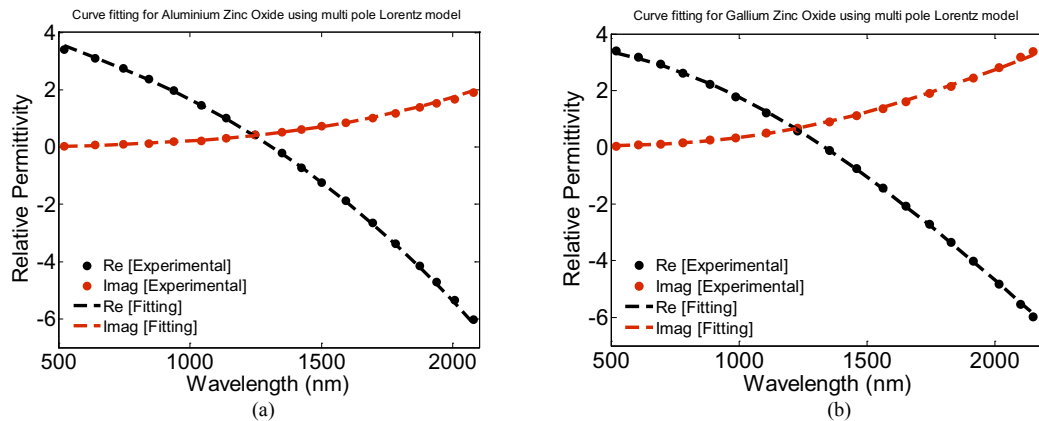


Fig. 2 Comparison of relative permittivity between our results and experimental values using Lorentz model for (a) AZO (b) GZO

5. Discussion and Conclusion

We have presented the Drude model parameters and multi pole Lorentz model parameters for low loss plasmonic materials, AZO and GZO. The optimized parameters are verified by comparing with the experimental results. To the best of our knowledge, the Drude model and the Lorentz model parameters of these materials have not been presented in any work till date. The parameters have been extracted using a nonlinear optimization algorithm based on the Nelder Mead method. The complex relative permittivities calculated using these parameters are in very good agreement with the experimental values over broad wavelength ranges. Since these parameters are applicable for broad frequency ranges, broadband calculation can be performed in a single run of the FDTD algorithm. Therefore, the algorithm utilizing these values will be computationally efficient compared to an algorithm using multi pole pair values. We also expect that this analysis will be helpful for the researchers to develop more accurate simulation models of low loss plasmonics materials.

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